Technical Manual of CCHE3D-GW

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**Table of Contents**

**CHAPTER 1 Introduction** .................................................................................................................. 2
  1.1 Background ................................................................................................................................ 2
  1.2 Capabilities of CCHE3D-GW ...................................................................................................... 3

**CHAPTER 2 Governing Equations and Boundary Conditions** ................................................................. 5
  2.1 Governing Equation ....................................................................................................................... 5
  2.2 Boundary Conditions and Initial Conditions ................................................................................ 7
    2.2.1 General-Head Boundary Condition ....................................................................................... 7
    2.2.2 River Boundary Condition .................................................................................................... 8
    2.2.3 Flux Boundary Condition ..................................................................................................... 9
    2.2.4 Active Well Boundary Condition ......................................................................................... 10

**CHAPTER 3 Numerical Methods** ...................................................................................................... 12
  3.1 Numerical Solution ....................................................................................................................... 12
  3.2 Finite Element Operators for CCHE3D-GW ............................................................................. 15
  3.3 Specific Input Files for CCHE3D-GW ......................................................................................... 18
    3.3.1 Input File for Basic Parameters .......................................................................................... 18
    3.3.2 Geo File for CCHE3D-GW ................................................................................................. 19
    3.3.3 Boundary Setting-up Module .............................................................................................. 20
    3.3.4 General-Head Condition Module ......................................................................................... 21
    3.3.5 River Boundary Module ...................................................................................................... 22
    3.3.6 Flux Boundary Module ........................................................................................................ 23
    3.3.7 Active Well Boundary Module ............................................................................................ 24
    3.3.8 Time-varying Aquifer Hydraulic Conductivity Module ..................................................... 25
    3.3.9 Hydraulic Properties Module .............................................................................................. 25
    3.3.10 Initial Condition Module ................................................................................................... 26

**CHAPTER 4 Verification of CCHE3D-GW** ......................................................................................... 27
  4.1 Verification of Dune-induced Hyporheic Flow ............................................................................ 27
    4.1.1 Conceptual Model ................................................................................................................. 27
    4.1.2 Simulation Domain and Mesh .............................................................................................. 28
    4.1.3 Case I: Pure Hyporheic Flow ............................................................................................... 30
    4.1.4 Case II: Hyporheic Flow with Base Flow ............................................................................ 31
    4.1.5 Case III: Hyporheic Flow under Two-layer Streambed ....................................................... 33
  4.2 Verification of Pumping in a Confined Alluvial Aquifer near a River ........................................ 34
  4.3 Verification of Pump in a Multiple-layer Aquifer ....................................................................... 41
    4.3.1 Case I: Steady State in Three-layer Aquifer ....................................................................... 41
    4.3.2 Case II: Steady State in Four-layer Aquifer ........................................................................ 44
    4.3.3 Case III: Transient State in Three-layer Aquifer ................................................................. 46
  4.4 Verification of Variably Saturated GW Flow ............................................................................. 48
    4.4.1 One-Dimensional Infiltration ............................................................................................... 49
CHAPTER 1 Introduction

1.1 Background

Groundwater (GW) is one of the most important resources for industries, agriculture, environment and civilization. The demand for more GW in recent decades has resulted in severe depletion worldwide. The exhaustion of GW resources has been a global problem. One example is the Mississippi River Valley Alluvial Aquifer in which GW declines have been constantly observed and reported over the last decades (Konikow, 2013). To mitigate this problem, the hydrological processes of the GW flow should be better understood so that wiser water resources management scheme can be proposed. Moreover, to evaluate the proposals for the GW resources management objectively, it is necessary to have decision-support tools that can precisely forecast the consequences from different scenarios. A process-based numerical model is one of the candidates that can fulfill the aforementioned requirements. By conceptualizing the detailed geophysical processes into proper governing equations and then solving them numerically, a numerical model can simulate a broad range of engineering problems efficiently and accurately, which can facilitate engineering design and decision-making.

For the GW flow models, MODFLOW has been widely used. It is a 3-D finite difference model developed by U.S. Geological Survey (USGS) (Langevin et al. 2017). Owing to the adopted governing equations, MODFLOW cannot simulate GW flows in partially saturated soils (vadose zone). On the other hand, the vadose zone is the area accommodating many activities related to GW hydrology, such as agricultural practices, rainfall infiltration and evapotranspiration. Therefore, it is essential to incorporate the vadose zone into the GW models. Moreover, the interaction between GW and surface water
(SW) has been a topic of interest in recent years, especially in the Mississippi River Alluvial Plain (Momm et al., 2022). Considering the close connection between the SW and GW, it is important to have an integrated surface-subsurface water model to enhance the understanding of the hydrological systems.

As a result, a 3-D finite element model, CCHE3D-GW, is developed based on the framework of CCHE3D (Jia et al., 2005; Jia et al., 2018), which is a surface water dynamic model developed by National Center for Computational Hydroscience and Engineering (NCCHE). In CCHE3D-GW, the mesh structure is the same as that in CCHE3D, so they are naturally compatible with each other, which will facilitate the future integrating work of SW and GW models. Additionally, CCHE3D-GW can simulate variably saturated GW flows, making it capable of handling flows in both fully saturated soils and vadose zone.

1.2 Capabilities of CCHE3D-GW

The present version of CCHE3D-GW has the following capabilities:

- It can simulate variably saturated GW flows because it uses the Richards equation (Richards 1931) as the governing equation. Thus, it can handle GW flows in both fully and partially saturated soils, i.e., the vadose zone has been considered in this model.

- CCHE3D-GW can handle various boundary conditions for GW flows, such as active wells (pumping or injection), general-head condition and flux boundary condition.

- In the present version of CCHE3D-GW, the SW dynamics, such as stream flow and infiltration, are considered as boundary conditions. Consequently, the GW-SW interactions are simulated by simplifying the SW flows as head or flux boundary
conditions. Although CCHE3D-GW has not been integrated with our SW models (CCHE2D/3D), the structure of mesh is the same as the one used in CCHE2D/3D, which will make it easier to integrate these SW and GW models in the future.

- For the simulation of GW-SW interactions, CCHE3D-GW can consider time-varying streambed conductivity, which is commonly encountered during flooding events (Korus et al., 2020; Levy et al., 2011; Mutiti and Levy, 2010; Zhang et al., 2011). This capacity is new for a GW numerical model.
CHAPTER 2 Governing Equations and Boundary Conditions

2.1 Governing Equation

One of the objectives of developing CCHE3D-GW is to simulate both saturated and unsaturated GW flows. Therefore, the Richards Equation, which was derived for the variably saturated GW flows, is used as the governing equation for CCHE3D-GW. The Richards Equation can be written in three forms, which are head-based, saturation-based and mixed. Among the three, the mixed form can produce a satisfactory mass balance both globally and locally (Celia et al. 1990). Thus, it is used to describe the GW flows in this model, which can be written as below:

\[
\frac{\partial \theta}{\partial t} + S \cdot S \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left[ K_x(\psi) \frac{\partial H}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K_y(\psi) \frac{\partial H}{\partial y} \right] + \frac{\partial}{\partial z} \left[ K_z(\psi) \frac{\partial H}{\partial z} \right] + q \tag{2.1}
\]

where \( H \) is hydraulic head (m); \( \psi \) is pressure head (= hydraulic head – elevation) (m); \( q \) represents sources and/or sinks of water (m\( \cdot \)s\(^{-1} \)), such as pump or injection; \( K_x, K_y \) and \( K_z \) are the \( x, y \) and \( z \) components of the hydraulic conductivity (m/s); \( S_s \) is specific storage (m\(^{-1} \)) and \( S = (\theta - \theta_r)/(\theta_s - \theta_r) \) is saturation (-) in which \( \theta \) is moisture content (m\(^3\)m\(^{-3} \)), \( \theta_r \) is residual moisture content (m\(^3\)m\(^{-3} \)) and \( \theta_s \) is saturated moisture content (m\(^3\)m\(^{-3} \)). When the pressure head (\( \psi \)) is larger than the air-entry pressure head (\( \psi_{air} \)), the soil is saturated. Under this condition, the moisture content (\( \theta \)) and hydraulic conductivity (\( K \)) are both of saturated values, and the saturation equals 1. When \( \psi \) becomes lower than \( \psi_{air} \), air enters soil, so the soil becomes unsaturated, which in turn reduces the values of \( \theta \) and \( K \), and makes the saturation less than 1.0. Moisture content and hydraulic conductivity of the unsaturated soil can be estimated from pressure head based on soil retention curves, which can be obtained by fitting the measured data with theoretical models (e.g., Brooks and Corey, 1966; van...
Genuchten, 1980). In the present version of CCHE3D-GW, two options are (Gardener 1958; van Genuchten, 1980) available to represent the soil retention curves (a.k.a. soil characteristic curves). The user can choose the preferred soil retention model through the input file. The formulas from Gardener (1958) are written as:

\[
\theta(\psi) = \theta_s + (\theta_s - \theta_r) e^{-\beta|\psi|}, \quad \psi < 0
\]  

(2.2a)

\[
\theta(\psi) = \theta_s, \quad \psi \geq 0
\]  

(2.2b)

\[
K(\psi) = K_s e^{-\alpha|\psi|}, \quad \psi < 0
\]  

(2.2c)

\[
K(\psi) = K_s, \quad \psi \geq 0
\]  

(2.2d)

The formulas of van Genuchten (1980) are written as:

\[
\theta(\psi) = \theta_s + \frac{(\theta_s - \theta_r)}{[1+(\alpha|\psi|)^{\frac{1}{\beta}}]^{1-\frac{1}{\beta}}}, \quad \psi < 0
\]  

(2.3a)

\[
\theta(\psi) = \theta_s, \quad \psi \geq 0
\]  

(2.3b)

\[
K(\psi) = K_s \frac{\left\{1-(\alpha|\psi|)^{\frac{1}{\beta}} \cdot \left[1+(\alpha|\psi|)^{\frac{1}{\beta}}\right]^{\frac{1}{\beta}}\right\}^2}{\left[1+(\alpha|\psi|)^{\frac{1}{\beta}}\right]^{\frac{1}{\beta+1}}}, \quad \psi < 0
\]  

(2.3c)

\[
K(\psi) = K_s, \quad \psi \geq 0
\]  

(2.3d)

where \(\alpha\) is a scaling parameter inversely related to the air-entry pressure, and \(\beta\) is a slope parameter inversely related to the pore-size distribution.
2.2 Boundary Conditions and Initial Conditions

Two commonly used boundary conditions, which are the general-head and flux boundary conditions, are covered by the present version of CCHE3D-GW. Additionally, two specific boundaries (river boundary and active wells) are included as well. The details are explained as follows.

2.2.1 General-Head Boundary Condition

The general-head boundary condition is set for the area with a known hydraulic head, such as lakes, ponds and a point with measured groundwater head data. Representative cases of this boundary condition is shown in Figure 2-1, and the mathematical formula is written as:

\[ H_{\text{at boundary}}(t) = H_b(t) \]  \hspace{1cm} (2.4)

where \( H_b(t) \) is the hydraulic head at the boundary, which can be measured GW depths (for the standing water such as lakes and ponds) or measured groundwater hydraulic heads. In the present version of CCHE3D-GW, the value of the hydraulic head in the general-head boundary can be either constant or time-variant, which is determined by the input file.

![Figure 2-1](image-url)  
*Figure 2-1. Two representative scenarios for the general-head boundary condition where (a) is for the standing water (such as lakes and ponds), and (b) is for the aquifer area with measured groundwater hydraulic heads.*
2.2.2 River Boundary Condition

One of the important aims of developing CCHE3D-GW is to provide the capability for future integration with the serial hydrodynamic models developed by NCCHE (CCHE-1D, 2D and 3D) so that the hydrological processes of the surface water-groundwater system can be simulated. Therefore, the river boundary condition is essential for CCHE3D-GW. A river can be represented by the general-head boundary in which the measured river stage is used for $H_b(t)$ in Eq. 2.4. However, real rivers are generally connected with aquifers through a low-permeable riverbed/riverbank which is not considered in Eq. 2.4. Thus, a specific river boundary condition is implemented in CCHE3D-GW, which can be written:

$$q_{at\text{-stream}} = \frac{C(t)}{L_n} \left[ H_{\text{stream}}(t) - H(t) \right]$$

(2.5)

where $H_{\text{stream}}(t)$ is the total head (= hydrostatic head + hydrodynamic head) of the surface water above the riverbed at time $t$, $L_n$ is the length of the river at the node, and $C(t)$ is streambed leakance (= streambed conductivity/streambed thickness).

Figure 2-2 shows the conceptual model of the river boundary condition. For a slow-moving river, its hydrodynamic heads are negligible so the measured time series of river stage can be used for $H_{\text{stream}}(t)$. For the situation that the river flow is fast (such as during flood events), $H_{\text{stream}}(t)$ can be simulated by process-based surface water models such as CCHE-1D, 2D or 3D. For the streambed leakance, many studies (Cui et al. 2021; Korus et al. 2020; Levy et al. 2011; Mutiti and Levy 2010; Schalchli 1992; Zhang et al. 2011) have revealed that it can change several orders of magnitude during flood events. Therefore, $C(t)$ can be set as a time-varying variable, and users can input its time series into the model. The constant streambed leakance option is also available in CCHE3D-GW to facilitate the study that the hydraulic properties of the streambed do not change too much.
2.2.3 Flux Boundary Condition

Figure 2-3 presents the flux boundary condition in which the boundary is located on the left. It is used to represent the condition that the discharge from a specific area to the aquifer is known, such as the measured exchange rate between a river and an adjacent aquifer, or the measured groundwater exchange flux between the studied aquifer and the surrounding aquifers. The mathematical formula is written as:

\[ q \big|_{\text{at boundary}} = K \cdot \nabla H \]  \hspace{1cm} (2.6)

where \( q \big|_{\text{at boundary}} \) is the prescribed flux at the boundary, and \( K \) is the hydraulic conductivity matrix. In the present version of CCHE3D-GW, the prescribed flux \( q \) needs to be disassembled into its \( x \), \( y \) and \( z \) components \( (q_x, q_y \text{ and } q_z) \) first (shown in Figure 2.3) by users and then input into the simulation. \( q_x, q_y \text{ and } q_z \) can be calculated as:

\[ q_x = K_{xx} \frac{\partial H}{\partial x} + K_{xy} \frac{\partial H}{\partial y} + K_{xz} \frac{\partial H}{\partial z} \]  \hspace{1cm} (2.7a)

\[ q_y = K_{yx} \frac{\partial H}{\partial x} + K_{yy} \frac{\partial H}{\partial y} + K_{yz} \frac{\partial H}{\partial z} \]  \hspace{1cm} (2.7b)

\[ q_z = K_{zx} \frac{\partial H}{\partial x} + K_{zy} \frac{\partial H}{\partial y} + K_{zz} \frac{\partial H}{\partial z} \]  \hspace{1cm} (2.7c)

As was shown in Eq. 2.1, in the present version of CCHE3D-GW, the hydraulic
conductivity matrix is diagonal because the principal directions of $K$ are assumed to be in line with normal $x$, $y$ and $z$ directions, i.e., only $K_{xx}$, $K_{yy}$ and $K_{zz}$ are non-zero in Eq. 2.7. Therefore, Eq. 2.7 can be simplified as:

$$q_s = K_{xx} \frac{\partial H}{\partial x}$$  \hspace{1cm} (2.8a)

$$q_y = K_{yy} \frac{\partial H}{\partial y}$$  \hspace{1cm} (2.8b)

$$q_z = K_{zz} \frac{\partial H}{\partial z}$$  \hspace{1cm} (2.8c)

2.2.4 Active Well Boundary Condition

Predictions of the effects of extraction and injection wells commonly must be made for GW management. It is therefore necessary to consider the active well boundary condition. Two scenarios have been included in the present version of CCHE3D-GW, which are the active well with a prescribed flux extraction/recharging rate and the active well with a prescribed head (Figure 2-4). The former active well is described by the sink/source term ($q$) in the governing equation (Eq. 2.1) in which a negative value is for extraction while a positive $q$ is for recharging. The latter active well can be represented by the general head boundary condition. The active well boundary can be set as constant or time-varying which is determined by the input file provided by users. It is also available
for users to set up the location of the well screen interval through the input file.

Figure 2-4. Conceptual model of well boundary condition where (a) is for the condition with a prescribed extraction/recharging flux rate, and (b) is for the condition with a prescribed head.
CHAPTER 3 Numerical Methods

3.1 Numerical Solution

A fully implicit numerical scheme and modified Picard’s iteration method (Celia et al. 1990) are adopted by CCHE3D-GW to solve the governing equation (Eq. 2.1) numerically. The fully implicit scheme is applied to provide a stable numerical solution, while the modified Picard’s iteration is used to linearize the non-linear equation owing to its reliability to achieve a convergent solution though it might be slower than more advanced approaches such as Gauss-Newton algorithm. Eq. 2.1 can then be re-written as:

\[
\frac{\theta^{m+1} - \theta^n}{\Delta t} + C^{m,n+1} \frac{H^{m+1,n+1} - H^{m,n+1}}{\Delta t} + S \cdot S_z \frac{H^{m+1,n+1} - H^n}{\Delta t} = \frac{\partial}{\partial x} \left[ K_x^{m,n+1}(\psi) \frac{\partial H^{m+1,n+1}}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K_y^{m,n+1}(\psi) \frac{\partial H^{m+1,n+1}}{\partial y} \right] + \frac{\partial}{\partial z} \left[ K_z^{m,n+1}(\psi) \frac{\partial H^{m+1,n+1}}{\partial z} \right] + q
\]

(3.1)

where \( C = \partial \theta / \partial H \), \( n \) is time step, and \( m \) is iteration step. For example, \( H^{m+1,n+1} \) represents the hydraulic head at the iteration step \( m+1 \) of the time step \( n+1 \).

A 3-D mixed form of control volume and finite element method is applied to solving Eq. 3.1 numerically. It is an extension of the 2-D method of Cumming et al. (2011). Suppose that the computational domain is discretized by \( N_x \times N_y \times N_z \) mesh points in which \( N_x, N_y \) and \( N_z \) represent the number of mesh points in x, y and z direction, respectively. The number of cells (control volumes) is therefore \((N_x - 1) \times (N_y - 1) \times (N_z - 1)\). For each control volume, the volumetric integration is conducted. With Gauss Divergence Theorem, Eq. 3.1 becomes:
where $V$ is a control volume, and $A_x$, $A_y$ and $A_z$ are the surface of $V$ with normal of $x$, $y$ and $z$ direction, respectively. In CCHE3D-GW, a structure mesh is adopted. Hydraulic head ($H$), hydraulic conductivity ($K_x$, $K_y$ and $K_z$) and moisture content ($\theta$) are located at the center of each control volume (cell) which is called a staggered node. The terms inside the surficial integration, i.e., $K_x(\psi)\frac{\partial H}{\partial x}$, $K_y(\psi)\frac{\partial H}{\partial y}$ and $K_z(\psi)\frac{\partial H}{\partial z}$ are the $x$, $y$ and $z$ components of Darcy velocity ($\mathbf{q}$). They are located at the vertex of a cell called a collocation node. Each collocation node is surrounded by eight hydraulic head nodes. The configuration of the mesh is shown in Figure 3-1. This mesh system is compatible with that of CCHE2D and 3D, making the work of integrating surface water and groundwater models much easier.

For each eight-neighbor hydraulic head node, the local coordinate ($\xi$, $\eta$ and $\zeta$) is built (shown in Figure 3-1), and the 3-D linear interpolation function is applied:

$$N_i = \frac{1}{8}(1 + \xi)(1 + \eta)(1 + \zeta)$$

(3.3)

where $i$ is the number of the hydraulic head node (from 1 to 8); $N_i$ is the linear interpolation function for each hydraulic head node; ($\xi_i$, $\eta_i$, $\zeta_i$) is the local coordinate of hydraulic head nodes and ($\xi$, $\eta$, $\zeta$) is the local coordinate of an arbitrary point inside the unit. The hydraulic head of an arbitrary point inside the unit can be computed as:

$$H = \sum_{i=1}^{8} (N_i \cdot H_i)$$

(3.4)

Therefore, the derivatives of hydraulic head in local coordinate can be calculated
as:

\[
\begin{align*}
\frac{\partial H}{\partial \xi} &= \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \xi} \cdot H_i \right), \\
\frac{\partial H}{\partial \eta} &= \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \eta} \cdot H_i \right), \\
\frac{\partial H}{\partial \zeta} &= \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \zeta} \cdot H_i \right)
\end{align*}
\]  

(3.5)

**Land Surface**

\[\nabla\text{ Water Table}\]

**Bottom of Aquifer**

Figure 3-1. Mesh configuration of CCHE3D-GW. Void circles represent the collocation nodes of the finite element mesh, and solid circles are staggered nodes. Darcy velocities are located on the collocation nodes, and hydraulic heads are located on staggered nodes. A cell consists of eight collocation nodes (void circles), and its center is the staggered node.

The derivatives of $H$ in global coordinates are obtained using standard finite element transformation. In the present version of CCHE3D-GW, these derivatives are only require to be computed at velocity nodes according to Eq. 3.2 so that the following equations can be derived for each unit:

\[
\begin{align*}
\frac{\partial H}{\partial x} &= \sum_{i=1}^{8} (a_{xi} \cdot H_i), \\
\frac{\partial H}{\partial y} &= \sum_{i=1}^{8} (a_{yi} \cdot H_i), \\
\frac{\partial H}{\partial z} &= \sum_{i=1}^{8} (a_{zi} \cdot H_i)
\end{align*}
\]  

(3.6)

where $a_{xi}$, $a_{yi}$ and $a_{zi}$ are the coefficients for each hydraulic head. Each unit contains one velocity node. The coefficient for each $H$ used to compute the Darcy velocity (derivatives
in the right-hand side of Eq. 3.2) is then obtained.

When calculating the new time step \( n+1 \), the variables \((H, \theta, K)\) at the old time step (time step \( n \)) have been obtained by the model, i.e., \( \theta^n \) and \( S^n \) are known in Eq. 3.2. For the new time step \( n+1 \), iterations are applied to achieve the convergent solution. When proceeding to the new iteration step \( m+1 \), the values at the old step (iteration step \( m \)) have all been computed, which means in Eq. 3.2, the values of \( H^{n,m+1}, \theta^{m,n+1}, K_x^{m,n+1}, K_y^{m,n+1}, K_z^{m,n+1} \) and \( C^{m,n+1} \) are all obtained, and the only unknown value is \( H^{m+1,n+1} \). Eq. 3.2 is therefore a linear equation for \( H^{m+1,n+1} \) and is solved by the strongly implicit procedure (SIP) method of Stone (1968). After getting the new value of \( H \), the latest values of \( \theta \) and \( K \) are computed from the constitutive equations (Eq. 2.2 or 2.3). The iteration will continue to update the value of \( H \) until the convergence criterion, \( \left| \frac{H^{n+1,n+1} - H^{m,n+1}}{H^{n+1}} \right| < \varepsilon \) (\( \varepsilon \) is a pre-determined small value, e.g., \( 1.0 \times 10^{-6} \)), is satisfied. When the convergence is achieved, the computation goes on to the next time step.

3.2 Finite Element Operators for CCHE3D-GW

Unlike the governing equation for the surface water flow (Navier-Stokes equation), the present numerical scheme to solving the Richards equation only needs the first-order derivative. Moreover, the primary variable in the GW governing equation is the hydraulic head rather than the velocity. As a result, the finite element operators used in CCHE3D-GW are slightly different from the SW module (CCHE3D), although the basic framework is the same.

As shown in Figure 3-2 (a), each element is composed of eight head nodes and one velocity node in which the velocity node (collocation node) is at the center of this element.
To represent the hydraulic head at any arbitrary point in the element, the 3-D linear interpolation function (Eq. 3.3) for each head node can be written as:

\[
N_i = \frac{1}{8} (1 - \xi)(1 + \eta)(1 - \zeta); \quad N_2 = \frac{1}{8} (1 - \xi)(1 - \eta)(1 - \zeta) \\
N_3 = \frac{1}{8} (1 + \xi)(1 - \eta)(1 - \zeta); \quad N_4 = \frac{1}{8} (1 + \xi)(1 + \eta)(1 - \zeta) \\
N_5 = \frac{1}{8} (1 - \xi)(1 + \eta)(1 + \zeta); \quad N_6 = \frac{1}{8} (1 - \xi)(1 - \eta)(1 + \zeta) \\
N_7 = \frac{1}{8} (1 + \xi)(1 - \eta)(1 + \zeta); \quad N_8 = \frac{1}{8} (1 + \xi)(1 + \eta)(1 + \zeta)
\]  

(3.7)

Because the collocation node is at the center of the element, its logical coordinate is (0.0, 0.0, 0.0). As a result, the hydraulic head at the collocation node can be represented by the hydraulic heads at the eight head nodes (Eq. 3.4). The derivative of the hydraulic head to the logical coordinates can then be written as Eq. 3.5. By using standard finite element transformation, the derivative of the hydraulic head to the physical coordinates can be written as:

\[
\left(\begin{array}{c}
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y} \\
\frac{\partial}{\partial z}
\end{array}\right) =
\left(\begin{array}{ccc}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\
\frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta}
\end{array}\right)^{-1}
\left(\begin{array}{c}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta} \\
\frac{\partial}{\partial \zeta}
\end{array}\right)
\]  

(3.8)

where

\[
\frac{\partial x}{\partial \xi} = \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \xi} \right) x_i; \quad \frac{\partial y}{\partial \eta} = \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \eta} \right) y_i; \quad \frac{\partial z}{\partial \zeta} = \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \zeta} \right) z_i \\
\frac{\partial y}{\partial \xi} = \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \xi} \right) y_i; \quad \frac{\partial y}{\partial \eta} = \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \eta} \right) y_i; \quad \frac{\partial y}{\partial \zeta} = \sum_{i=1}^{8} \left( \frac{\partial N_i}{\partial \zeta} \right) y_i
\]

(3.9)

The coefficients for the hydraulic gradient in the physical coordinate (Eq. 3.6) can therefore be obtained. These finite element operators and transformations are programmed
in the subroutines ‘ELMTP_GW_2D’, ‘ELMTP_GW_3D’ and ‘ELMTP_GW_3D_NEW’, which are all included in the module ‘GW_OPRT_UNSATURATED.f90’. After attaining the coefficients for the hydraulic gradients, with Darcy’s law the GW velocity passing through the surface of each control volume (Figure 3-2b) can be calculated. The surficial integration in the governing equation (Eq. 3.2) can therefore be computed based on Gaussian integration, which can be written as:

\[
\int_{\Gamma} \left[ K_{m,n}^{(m+1,n+1)}(\psi) \frac{\partial H}{\partial x} \right] dA_x \approx \left[ K_{m,n}^{(m+1,n+1)}(\psi) \frac{\partial H}{\partial x} \right] \Delta A_x \\
\int_{\Gamma} \left[ K_{m,n}^{(m+1,n+1)}(\psi) \frac{\partial H}{\partial y} \right] dA_y \approx \left[ K_{m,n}^{(m+1,n+1)}(\psi) \frac{\partial H}{\partial y} \right] \Delta A_y \\
\int_{\Gamma} \left[ K_{m,n}^{(m+1,n+1)}(\psi) \frac{\partial H}{\partial z} \right] dA_z \approx \left[ K_{m,n}^{(m+1,n+1)}(\psi) \frac{\partial H}{\partial z} \right] \Delta A_z
\]

(3.10)

where \(\Delta A_x, \Delta A_y\) and \(\Delta A_z\) define the area of the plane with the normal in \(x, y\) and \(z\) direction, respectively (Figure 3-2b). These surficial areas are calculated in the subroutine ‘SUFINIT_GW’. The numerical surficial integrations are conducted in the subroutine ‘PRESSURE_GW1’. The harmonic average is used to compute the hydraulic conductivity \((K_x, K_y \text{ and } K_z)\) in Eq. 3.10.

Figure 3-2. Mesh configuration of CCHE3D-GW where (a) is the logical coordinate for an element, and (b) displays a control volume.
3.3 Specific Input Files for CCHE3D-GW

GW and SW models have different parameters, so the input files for CCHE3D-GW differ from the SW modules. The specific modules that are designed to address these specific input files will be explained in the rest of section 3.3.

3.3.1 Input File for Basic Parameters

The input file for setting up the basic parameters for the simulation is named ‘basic_input.dat’. Figure 3-3 shows the structure of this file.

![Figure 3-3. Format of the input file for the basic parameters.](image)

- In the first record, IMAX, JMAX, KMAX are the maximum numbers of the head nodes in x, y and z direction, respectively.

- In the second record, T_LIM is the ending time for the simulation. DT is time step. DT_AMP is the amplification factor for DT at each time step, which makes the actual time step be (Initial Time Step × DT_AMP^(Number of Time Steps)). T_START is the starting time of the simulation.

- In the third record, NCYC_OUT is an integer interval used to control how many time steps to output simulation results. For instance, if NCYC_OUT is set to 10, the simulation results will be written every 10 time steps. NCYC_CHECK is used
to control how many steps the model shows the user the condition of the convergence. For example, if NCYC_CHECK is equal to 5, the model will display the maximum $\frac{|H_{m+1,n+1} - H_{m,n}|}{H_{m,n}}$ to the user each five time steps.

- In the fourth record, UIT is used to determine the soil characteristic models in which UIT = 1 is set for the model of van Genuchten (1980), and UIT = 2 is for the model of Gardner (1958).
- In the fifth record, ERRO.Inner is the tolerance of the SIP method, and ERRO.Total is the tolerance of the modified Picard’s iteration.
- In the sixth record, Z0 is the vertical coordinate of the datum.
- In the seventh record, WELL_Num is the number of active wells. HEAD_Num is the number of general-head boundary conditions. FLUX_Num is the number of flux boundary conditions. RIVER_Num is the number of river boundary conditions.
- In the eighth record, K_VAR determines whether the hydraulic conductivity of the aquifer will be changed over the simulation period. For this parameter, a value of ‘0’ indicates constant aquifer hydraulic conductivity, and ‘1’ indicates the time-varying condition. When this parameter is turned on (= 1), the module that can change the aquifer hydraulic conductivity (described in subsection 3.3.8) will be activated.
- In the ninth record, INNER_Control determines the maximum number of SIP iterations.

3.3.2 Geo File for CCHE3D-GW

The input file to setting up the mesh for the simulation is named ‘case_name.geo’.
Figure 3-4 shows the structure of this file.

<table>
<thead>
<tr>
<th>IMAX, JMAX, KMAX</th>
</tr>
</thead>
<tbody>
<tr>
<td>X_Coordinate, Y_Coordinate, Top_ELV, Bottom_ELV, Boundary_TYPE, Manning</td>
</tr>
</tbody>
</table>

Figure 3-4. Format of the Geo file for CCHE3D-GW.

The format of the Geo file for CCHE3D-GW is generally the same as the file for CCHE3D. The only differences are the following:

- Unlike SW flow, GW is constrained in the subsurface area, so the vertical domain is defined by the elevation of the top (Top_ELV) and the bottom (Bottom_ELV).

- The boundary types are much more complicated in the GW flows than in the SW. Therefore, the parameter ‘Boundary_TYPE’, which is used to determine the type of the mesh node in the SW models, is only preserved to be consistent with the format of the Geo files in the CCHE2D/3D (SW models). This value is not used by CCHE3D-GW.

- The GW does not have Manning’s coefficient, but this parameter ‘Manning’ is still preserved here to be compatible with the SW models. This value is not used by CCHE3D-GW.

3.3.3 Boundary Setting-up Module

As was mentioned in section 3.3.2, the boundary types for the GW flow are much more complex than the SW. Therefore, the boundary types in CCHE3D-GW are set up by separate files which are explained below.

- The file ‘nf.dat’ is used to separate the inner and the boundary nodes where nf = 0 is for an inner node, and nf = 1 is for a boundary node.

- The files ‘kl.dat’, ‘kr.dat’, ‘ks.dat’, ‘kt.dat’, ‘kn.dat’, ‘kb.dat’ and ‘kt.dat’ are the
input files defining the left, right, front (south), back (north), bottom and top boundary conditions for each control volume, respectively. These boundary (flag) parameters are all integers in which ‘1’ is used for the general-head condition; ‘2’ is for the river boundary condition; ‘4’ is used for the flux condition.

- In CCHE3D-GW, the 3-D array (all of the aforementioned boundary parameters are 3-D array) is read in the following format:

  For \( k = 1, k_{\text{max}} \)
  
  For \( j = 1, j_{\text{max}} \)
  
  Read \( \text{Array}(i, j, k), i = i_{\text{max}} \)

  where \( i, j \) and \( k \) are indices in \( x, y \) and \( z \) direction, respectively.

3.3.4 General-Head Condition Module

The input file to set up the general-head condition is named ‘head+number.bound’.

For instance, the number five head boundary file is named as ‘head5.bound’. Figure 3-5 shows the format of this file.

![Figure 3-5](image)

Figure 3-5. Format of the input file for general-head condition where (a) is for constant head, and (b) is for time-varying head.

- The first record (ITYPE) determines whether it is a constant (= 0) or a time-varying (≠ 0) head condition.
- From the second to fourth records, I_START, J_START and K_START are the starting indices of the general-head boundary in the \( x, y \) and \( z \) directions, respectively. I_END, J_END and K_END are the ending indices of the general-
head boundary in the $x$, $y$ and $z$ directions, respectively.

- In the fifth record, when it is a constant head condition (ITYPE = 0), only the prescribed hydraulic head (H_PREScribed) will be read by the model. For the time-varying head condition, the time series that include time (H_TIME) and prescribed head value (H_PREScribed) will be read by the program. The input H_TIME is usually not identical to the simulation time step, so a simple linear interpolation is built in the model to obtain the hydraulic head in each simulation time step based on this input data.

3.3.5 River Boundary Module

The input file to set up the river boundary condition is named ‘river+number.bound’. For instance, the number seven river boundary file is named as ‘river7.bound’. Figure 3-6 shows the format of this file.

- The first record (ITYPE) determines whether it is a constant (= 0) or a time-varying (≠ 0) river condition. Either a time-varying river stage or a time-varying streambed conductivity should be defined as a time-varying river boundary.

- From the second to fourth records, I_START, J_START and K_START are the starting indices of the river in the $x$, $y$ and $z$ directions, respectively. I_END, J_END and K_END are the ending indices of the river in the $x$, $y$ and $z$ directions, respectively.

- Starting from the fifth record, when it is a constant river condition (ITYPE = 0), only one column will be read. Parameters are defined as follows: RIVER_STAGE is the measured river stage; STREAMBED_CONDUCTIVITY is streambed conductivity; STREAMBED_THICKNESS is the thickness of the streambed;
RIVER_CELL_AREA is the area of the river on the surface of this control volume. RIVER_CELL_AREA can be smaller than the surficial area of the control volume representing that the control volume is only partially occupied by the river. For the time-varying river boundary, the time series will be read in the following records in which RIVER_TIME is the time. Because the input RIVER_TIME is usually not identical to the simulation time step, a simple linear interpolation is adopted to compute the river stage in each simulation time step. For the streambed conductivity, the linear interpolation is conducted for its natural logarithmic value.

<table>
<thead>
<tr>
<th>ITYPE (= 0, Constant River Stage)</th>
<th>(a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I_START, I_END</td>
<td></td>
</tr>
<tr>
<td>J_START, J_END</td>
<td></td>
</tr>
<tr>
<td>K_START, K_END</td>
<td></td>
</tr>
<tr>
<td>RIVER_HEAD, STREAMBED_CONDUCTIVITY, STREAMBED_THICKNESS, RIVER_CELL_AREA</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ITYPE (NOT EQUAL TO 0, Time-varying River Stage)</th>
<th>(b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I_START, I_END</td>
<td></td>
</tr>
<tr>
<td>J_START, J_END</td>
<td></td>
</tr>
<tr>
<td>K_START, K_END</td>
<td></td>
</tr>
<tr>
<td>RIVER_TIME, RIVER_HEAD, STREAMBED_CONDUCTIVITY, STREAMBED_THICKNESS, RIVER_CELL_AREA</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3-6. Format of the input file for river boundary condition where (a) is for constant river stage, and (b) is for time-varying river stage or streambed conductivity.

3.3.6 Flux Boundary Module

The input file to set up the flux boundary condition is named ‘flux+number.bound’. For instance, the number six flux boundary file is named as ‘flux6.bound’. Figure 3-7 shows the format of this file.

- The meanings of the parameters in the first four records are the same as those in the general-head boundary file (Figure 3-5).

- Starting from the fifth record, when it is a constant flux condition (ITYPE = 0), only one column will be read. LEFT_FLUX, RIGHT_FLUX, FRONT_FLUX,
BACK_FLUX, BOTTOM_FLUX and TOP_FLUX are prescribed fluxes from left, right, front, back, bottom and top faces of the control volume, respectively. For the time-varying flux boundary, the time series will be read in the following records in which FLUX_TIME is the time. Because the input FLUX_TIME is usually not identical to the simulation time step, a simple linear interpolation is adopted to calculate the flux from the input data in each simulation time step.

(a)

<table>
<thead>
<tr>
<th>ITYPE ((= 0), Constant Flux)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I_START, I_END</td>
</tr>
<tr>
<td>J_START, J_END</td>
</tr>
<tr>
<td>K_START, K_END</td>
</tr>
<tr>
<td>LEFT_FLUX, RIGHT_FLUX, FRONT_FLUX, BACK_FLUX, BOTTOM_FLUX, TOP_FLUX</td>
</tr>
</tbody>
</table>

(b)

<table>
<thead>
<tr>
<th>ITYPE (NOT EQUAL TO 0, Time-varying Flux)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I_START, I_END</td>
</tr>
<tr>
<td>J_START, J_END</td>
</tr>
<tr>
<td>K_START, K_END</td>
</tr>
<tr>
<td>FLUX_TIME, LEFT_FLUX, RIGHT_FLUX, FRONT_FLUX, BACK_FLUX, BOTTOM_FLUX, TOP_FLUX</td>
</tr>
</tbody>
</table>

Figure 3-7. Format of the input file for flux boundary condition where (a) is for constant flux, and (b) is for time-varying flux.

3.3.7 Active Well Boundary Module

The input file to set up the active well boundary condition is named ‘well+number.bound’. For instance, the file for the number one injection/pumping well is named as ‘well1.bound’. Figure 3-8 shows the format of this file. The structure and meanings of these parameters are the same as the general-head boundary file. The only thing needs to be mentioned is that the volumetric rate should be assigned by a positive sign for the injection well, while it should be a negative value for the pumping well in CCHE3D-GW.
3.3.8 Time-varying Aquifer Hydraulic Conductivity Module

The hydraulic conductivity of the aquifer might change with time owing to geophysical and chemical processes, such as clogging and soil erosion. To consider these factors, the time-varying aquifer hydraulic conductivity module can be activated by setting K_VAR to 1 in the ‘basic_input.dat’ (Figure 3-3). The input file to set up the time-varying aquifer hydraulic conductivity is named ‘aquifer+number.bound’. Figure 3-9 shows the format of this file. The structure and meanings of these parameters are similar the same as the general-head boundary file. In Figure 3-9, K_TIME and NEW_K_Value are the time and the new value of the aquifer hydraulic conductivity, respectively.

3.3.9 Hydraulic Properties Module

The soil properties are defined by Eq. 2.2 or Eq. 2.3 in which the input parameters $\theta_r$, $\theta_s$, $K_s$, $\alpha$ and $\beta$ are defined by input files ‘thetar.dat’, ‘thetas.dat’, ‘k_s.dat’, ‘alpha.dat’ and ‘m2.dat’, respectively. The specific storage of the aquifer is determined by ‘ss.dat’. All
of these parameters are 3-D arrays, so the reading format described in section 3.3.3 is used.

3.3.10 Initial Condition Module

The initial hydraulic head is input to the model through the file ‘head_initial.dat’.

It is also a 3-D array, so the reading format in section 3.3.3 is used.
CHAPTER 4 Verification of CCHE3D-GW

Verification is an imperative step for a newly developed numerical model because it can prove the applicability of the model. It is preferable to use analytical solutions that are similar to the real world problems as verification cases so that both the mathematical and physical correctness can be examined simultaneously. The verification results of the newly developed CCHE3D-GW are shown in this chapter. The following cases were chosen for the verification, which are (1) dune-induced hyporheic flow (fully saturated GW flow); (2) pumping in a confined alluvial aquifer near a river (fully saturated GW flow); (3) pumping in a multiple-layer aquifer (fully saturated GW flow); (4) 1-D infiltration in an initially unsaturated soil (variably saturated GW flow) and (5) pump in an unconfined aquifer which includes the vadose zone (variably saturated GW flow).

4.1 Verification of Dune-induced Hyporheic Flow

4.1.1 Conceptual Model

Dunes in rivers promote hyporheic exchange because of the dynamic pressure difference on its stoss and lee sides (Figure 4-1a). To facilitate the verification, this dune-induced hyporheic flow was simplified to be a vertical 2-D case in which the streambed was assumed to be flat considering that the dune height usually is small compared to the dune length (Figure 4-1b). Under this simplification, the pressure distributions along natural triangular dunes were found to generally follow a sinusoidal function (Elliot and Brooks 1997a and b). The boundary condition of this problem can therefore be written as:

\[ H(x,0) = H_m \cos \left( \frac{2\pi x}{L} \right) + x \]  

(4.1a)
where $L$ is the wavelength of a dune, $s$ is streambed slope; $D$ is thickness of the alluvium in which the $z$ coordinate is set up downward; $q_b$ is the quantity of base flow flux where the sign ‘±’ is used for gaining and losing condition, respectively; $H_m$ is amplitude of the hydraulic head distribution which is computed by an empirical formula from Shen et al. (1990):

\[
H_m = 0.28 \frac{V^2}{2g} \left\{ \begin{array}{ll}
\frac{\Delta}{0.34H_s}^{3/8}, & \text{if } \frac{\Delta}{H_s} \leq 0.34 \\
\frac{\Delta}{0.34H_s}^{3/2}, & \text{if } \frac{\Delta}{H_s} > 0.34
\end{array} \right. 
\]  

(4.2)

where $\Delta$ is dune height, $H_s$ is stream water depth, $g$ is gravitational acceleration ($= 9.81 \text{ m/s}^2$) and $V$ is mean stream flow velocity.

4.1.2 Simulation Domain and Mesh

Dunes with the wavelength of 1.0 m and height of 0.08 m were set up for the verification. The thickness of the domain was 1.0 m, and the length in $x$ direction was 3.0 m, covering three dunes. The results of the middle dune were chosen for analysis to minimize boundary effects. This domain was discretized by a uniform mesh with $\Delta x = \Delta z = 0.005 \text{ m}$. For the hydrological parameters, the steady mean stream velocity was set to 0.129 m/s, and the stream water depth was 0.4 m. As a result, $H_m$ was computed to be 0.0134 m from Eq. 4.2.
Figure 4-1. (a) Configuration of the dune-induced hyporheic flow in the longitudinal view; (b) conceptual model of this verification case; the transverse view of the dune-induced hyporheic flow under (c) gaining and (d) losing condition.

Figure 4-2. Simulation domain of the 2-D dune-induced hyporheic flow in which the upper sediment layer is marked in grey, and the lower layer is in white.
Figure 4-2 summarizes the configuration of the numerical simulations for the verification. The datum was set at the streambed surface, and the sinusoidal hydraulic head distribution was directly imposed on the top boundary. The left and right boundaries were both set as a constant flux. The base flow was represented by the bottom boundary condition.

4.1.3 Case I: Pure Hyporheic Flow

The first case is the scenario that only the hyporheic flow driven by the head gradient along the streambed surface exists, i.e., both $s$ and $q_b$ are zero. Under this simplified condition, an analytical solution was derived by Packman et al. (2000) which can be written as:

$$H(x, z) = H_0 \cos(\lambda x) \left[ \tanh(\lambda D) \cdot \sinh(-\lambda z) + \cosh(-\lambda z) \right]$$

(4.3)

Figure 4-3. Comparisons between simulation results and analytical solution for hydraulic head distributions at four vertical layers in which (a) is at $z = -0.01$ m, (b) is at $z = -0.11$ m, (c) is at $z = -0.21$ m and (d) is at $z = -0.31$ m.
The hydraulic heads computed from the analytical solution and CCHE3D-GW were compared at four representative layers (Figure 4-3). It can be found that the values of $R^2$ are all high (0.99) at these four layers, indicating a very good agreement between the results from the numerical model and the analytical solution. Therefore, CCHE3D-GW is proven applicable for this case.

4.1.4 Case II: Hyporheic Flow with Base Flow

The ambient GW flows, such as underflow and base flow, often concur with the hyporheic flow. Open channel flow is driven by the energy slope which can propagate in the shallow alluvial aquifer, resulting in a general horizontal GW flow, called underflow. The underflow can be represented by Eq. 4.1b mathematically. Additionally, the river water surface elevation is generally different from the GW table, which therefore causes the hydraulic gradient between them (Figure 4-1 c and d). Consequently, the base flow is formed which can be formulated by Eq. 4.1c. For the scenario that the dune-induced hyporheic flow occurring with both underflow and base flow, an analytical solution was derived by Marzadri et al. (2016), which can be written as:

$$H(x, z) = H_m \cos(\lambda x) \left[ \tanh(\lambda D) \sinh(\lambda z) + \cosh(\lambda z) \right] - sx \mp \frac{q_b}{K} z \quad (4.4)$$

For this verification case, $q_b$ was set to 0.020 m/d and $s$ was 0.01%. Good agreements between the simulated and analytical hydraulic head distributions can be found for both gaining (Figure 4-4) and losing (Figure 4-5) conditions, demonstrating the capability of CCHE3D-GW in handling base flow boundary conditions.
Figure 4-4. Comparisons between simulated and analytical hydraulic head distributions for gaining condition at four vertical layers in which (a) is at $z = -0.01$ m, (b) is at $z = -0.11$ m, (c) is at $z = -0.21$ m and (d) is at $z = -0.31$ m.

Figure 4-5. Comparisons between simulated and analytical hydraulic head distributions for losing condition at four vertical layers in which (a) is at $z = -0.01$ m, (b) is at $z = -0.11$ m, (c) is at $z = -0.21$ m and (d) is at $z = -0.31$ m.
4.1.5 Case III: Hyporheic Flow under Two-layer Streambed

The first two cases are for a homogenous aquifer while layered aquifers are common in the real world as well. Therefore, it is necessary to verify the numerical model under such a circumstance. An analytical solution was derived by Marion et al. (2008) for a two-layer streambed to study the effects from an armor-layer sediment. The simulation domain consisted of two layers, which was an upper layer with a thickness of $D_u$ and a hydraulic conductivity of $K_u$, and a lower layer with a thickness of $D_l$ and a hydraulic conductivity of $K_l$ (Figure 4-2). In this verification case, $K_u$ and $K_l$ were set to 65.26 m/day and 6.526 m/day, respectively. $D_u$ and $D_l$ were set to 0.16 m and 0.84 m, respectively. The ambient GW flows were not considered, i.e., both $s$ and $q_b$ were zero. The rest of the parameters were the same as the case I. The analytical solution is written as:

$$\begin{align*}
H(x, z) &= H_m \cos(\lambda x) \frac{\sinh \left[ \lambda (D_u + z) \right] - h_{12} / H_m \sinh (\lambda D_u)}{\sinh (\lambda D_u)}, \quad -D_u < z < 0 \quad (4.5a) \\
H(x, z) &= H_{12} \cos(\lambda x) \frac{\cosh \left[ \lambda (D_u + D_l + z) \right]}{\cosh (\lambda D_l)}, \quad -(D_u + D_l) < z < -D_u \quad (4.5b)
\end{align*}$$

where $H_{12}$ is the intermediate hydraulic head between the upper and lower layers, and it is computed as:

$$H_{12} = \frac{\csc h (\lambda D_u)}{\coth (\lambda D_u) + K_i / K_u \tanh (\lambda D_l)} \quad (4.6)$$

Good agreements between the simulated and analytical hydraulic head distributions can be found (Figure 4-6), revealing that CCHE3D-GW is able to simulate the GW flows under this two-layer streambed condition.
Figure 4-6. Comparisons between simulated and analytical hydraulic head distributions for a two-layer streambed with $K_u = 65.26$ m/day, $K_l = 6.526$ m/day, $D_u = 0.16$ m and $D_l = 0.84$ m at four vertical layers: (a) $z = -0.01$ m, (b) $z = -0.11$ m, (c) $z = -0.21$ m and (d) $z = -0.31$ m.

4.2 Verification of Pumping in a Confined Alluvial Aquifer near a River

Pumping a well adjacent to a river to induce infiltration of SW into an aquifer is a method often used for acquiring source water for drink water supply or managed aquifer recharge (Tufenkji et al. 2002; O’Reilly et al. 2022). As a result, it is beneficial to examine whether the newly developed CCHE3D-GW can simulate this processes. Owing to the complexity of the variably saturated GW flows, few analytical solutions have been derived for pumping near a river with the consideration of the vadose zone. Therefore, the analytical solution of Butler et al. (2001), which was derived for the near-river pump in a confined aquifer (the GW flows are therefore fully saturated), was chosen for the verification.
To derive the analytical solution, the problem was conceptualized as a depth-averaged 2D flow system (Figure 4-7) in which the GW flow properties in the vertical direction were assumed uniform, and the vertical flow was neglected. The pumping well fully penetrated the alluvial aquifer, and it was placed near a river. The river was represented as a constant head boundary condition in this analytical model. The cross section of the river was idealized to be rectangular. The riverbank was impermeable, but the riverbed can transmit the water flux between the stream and the aquifer. The hydraulic conductivity of the overlying confining unit (aquitard) was assumed zero, and there was no flow at the lateral boundaries or base of the aquifer. The domain was therefore divided into three zones: Zone 1 was the aquifer on the left of the river containing the pumping well, Zone 2 was the aquifer beneath the riverbed, and Zone 3 was the aquifer on the right side. \( T_i \) and \( S_i \) were used to represent transmissivity and storativity of these zones, respectively. The properties of these zones can be different, but they were homogeneous in one zone. Figure 4-7b shows the coordinate system in which the origin was located at the pumping well.

Figure 4-7. The conceptual model of Butler et al. (2001) where (a) is the view of the cross section passing the pumping well and perpendicular to the river, and (b) is the \( x - y \) plane view. The four red dashed lines in Figure 4-7(a) are the representative locations for the comparisons in Figure 4-9.
The domain of the verification cases was 20,300 m × 28,600 m, discretized by a non-uniform mesh (138 × 139 grid cells in x and y directions). Coarser meshes were applied to the region far from the pumping well, and the near field was represented by fine and uniform meshes (2 m × 2 m) (Figure 4-8). The width of river, w, was 42 m, and the thickness of riverbed, b’, was assumed 2 m. The pumping well was set fully penetrating the aquifer, and the pumping rate, Q, was 12,960.0 m³/day. The aquifer was 40 m thick. The transmissivities of the three zones, T₁, T₂ and T₃, were all assumed 2400 m²/day, and aquifer storativity (S₁, S₂ and S₃) was 0.12 m. The relative permeability of riverbed was reflected by a dimensionless parameter, B:

\[ B = \frac{K_r \cdot w^2}{b' \cdot T_2} \]  \hspace{1cm} (4.7)

where \( K_r \) is streambed conductivity.
Multiple scenarios were simulated to cover a variety of parameters. The values of streambed conductivity are listed in Table 4-1, and the streambed leakance was computed from Eq. 4.7. For each case, the initial time step, Δt, was 0.001 days, and it was increased by a factor of 1.1 in each step. The total simulation time was 138 days. The initial hydraulic head of the aquifer was set as 50 m to ensure the aquifer was fully saturated during the pumping process. The river stage was set to be constant, 50 m, in all simulations.

CCHE3D-GW was verified using a 4-layer mesh and a 12-layer mesh. With more layers in z direction, 3D groundwater flow features can be better simulated. The setup of the 4-layer mesh fits exactly as that of the depth-averaged 2D analytical solution because
the vertical flow in the solution is technically minimal. When the 12-layer mesh was tested, the hydraulic conductivity in $z$ direction ($K_z = 2000$ m/day) was set much larger than those of the horizontal directions ($K_x, K_y = 60$ m/day) so that the vertical gradient of the GW flow was negligible compared to the other two directions. Consequently, the simulated GW flow behaves like 2D, which makes the simulation results comparable to the analytical solution.

| Table 4-1. The Parameters of Verification Cases |
|-----------------|-----------------|
| $B [-]$         | Streambed Conductivity $k_r$ (m/day) |
| Case 1          | 0.001           | 0.00272       |
| Case 2          | 0.1             | 0.272         |
| Case 3          | 1.0             | 2.72          |
| Case 4          | 10.0            | 27.2          |
| Case 5          | 100.0           | 272           |

Two parameters, dimensionless drawdown ($\Phi$) and stream depletion ($\Delta Q$) were used for comparisons between the simulated and analytical results, which can be written as:

$$\Phi_i = \frac{d_i \cdot T_i}{Q} \quad (4.8a)$$

$$\Delta Q = \frac{\Delta q}{Q} \quad (4.8b)$$

where $d_i$ is drawdown in Zone $i$ ($H - H_i |_{t=0}$), and $\Delta q$ is discharge from river to aquifer.

Figure 4-9a – d are the comparisons of the simulated and analytical drawdown curves at four representative locations (red dashed lines in Figure 4-7a) in the cross section passing the pumping well and perpendicular to the river. Each of the sub-figures has five groups of curves, representing the five cases in Table 4-1, computed by 4-layer mesh, 12-layer mesh and the analytical model. Figure 4-9e shows the comparisons for the dimensionless stream depletion. Fine agreements are found between the numerical results
and the analytical solutions, and between the results of the 4-layer and 12-layer meshes, verifying the capability of CCHE3D-GW in simulating the pump near an alluvial river. When the riverbed is almost impermeable \( B = 0.001 \), the river does not respond much to the pump, and the solution becomes identical to that of Theis (1935), i.e., the drawdown increases and approaches infinite with the pumping time. Under this circumstance, the stream depletion keeps minimal during the whole process. With a permeable riverbed (Case 2 - 5), the drawdown increases at the beginning but slows down at a certain time. Under these conditions, the stream depletion grows with different rates depending on the values of riverbed permeability. When the stream depletion approaches 1, the extracted water is completely balanced by the discharge from river, and drawdown of the aquifer ceases. With the increase of the streambed leakance (from Case 2 to 5), the equilibrium condition is achieved earlier, and the stabilized drawdown value is smaller (Figure 4-9).
Figure 4-9. Comparisons of drawdown between the results of analytical solution (Butler et al., 2001) and CCHE3D-GW with 4 layers and 12 layers in $z$ direction where $x/w$ (a) = 0.523 (Zone 1); (b) = -0.429 (Zone 1); (c) = -1.238 (Zone 2) and (d) = -3.425 (Zone 3). (e) Comparisons of stream depletion between the results of analytical solution (Butler et al., 2001) and CCHE3D-GW with 4 layers and 12 layers in $z$ direction with different streambed leakances.
4.3 Verification of Pump in a Multiple-layer Aquifer

The verification case in 4.2 is for a pump in a single-layer aquifer. However, in real-world problems, multiple-layer aquifers are commonly encountered as well. Thus, in this subsection CCHE3D-GW is verified with a series of analytical solutions derived by Motz and Acar (2007) and Hemker (1985) which deals with pumping from a single aquifer in the multiple-layer aquifer. The analytical solutions represent steady-state or transient conditions and assume horizontal flow only in the aquifers and vertical flow only in the confining units.

4.3.1 Case I: Steady State in Three-layer Aquifer

The three-layer aquifer for this verification is located at Titusville/Mims area, which is in the northern part of Brevard County, Florida. The whole system is composed of three aquifers, which are surficial aquifer, Upper Floridan aquifer and Lower Floridan aquifer (Figure 4-10). For this steady state, the storativity of the aquifer ($S_i$) was zero while the transmissivity of each aquifer ($T_i$) was listed in table 4-2. The pumping well was located in the Upper Floridian aquifer with a pumping rate $Q$ of 353,000 ft$^3$/day. These three aquifers are separated by confining units which, given the steady-state conditions and large disparity in hydraulic conductivity compared to the aquifers, were simulated by a leakance value. Leakance is the ratio of the hydraulic conductivity ($K_v$) and the thickness ($b$) and specified values can be found in Table 4-2. On top of the surficial aquifer, an evapotranspiration layer was imposed to represent the exchange of the GW and the atmosphere. In this vertical direction ($z$), seven layers were set in the simulations with CCHE3D-GW. Because transmissivity and leakance values were used for aquifers and confining units, respectively, each layer was set to 1.0 ft thick for convenience.
In the lateral plane ($x$ - $y$) the simulation domain was 721,826 ft $\times$ 721,826 ft which was sufficiently large to eliminate the effects from lateral boundaries. The origin of the $x$ - $y$ coordinates was set at the pumping well, which was the center of the domain. The simulation domain was discretized by 139 $\times$ 139 mesh grids in the $x$ – $y$ plane in which a uniform mesh ($\Delta x = \Delta y = 100$ ft) was used from $x = -2500$ ft to 2500 ft and $y = -2500$ ft to 2500 ft, and a non-uniform mesh with an amplification factor of 1.15 was applied to the remaining domain (Figure 4-11). The lateral boundary conditions were all set to a constant head (15.0 ft). The initial GW head for the simulation was set to 15.0 ft.

![Diagram of the three-layer aquifer system](image)

---

**Figure 4-10.** Conceptual model of the pump in the three-layer aquifer.
Table 4-2. Hydraulic Properties of Each Layer for the Three-layer Aquifer Simulation

<table>
<thead>
<tr>
<th>Hydrogeological Units</th>
<th>Layer Number</th>
<th>Hydraulic Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top Boundary Unit</td>
<td>7</td>
<td>Constant head $H = 15.0$ ft</td>
</tr>
<tr>
<td>Evapotranspiration Reduction</td>
<td>6</td>
<td>$(K_b/b) = 1.52 \times 10^{-4}$ day$^{-1}$</td>
</tr>
<tr>
<td>Surficial Aquifer</td>
<td>5</td>
<td>$T_1 = 1.000$ ft$^2$/day</td>
</tr>
<tr>
<td>Intermediate Confining Unit</td>
<td>4</td>
<td>$(K_b/b) = 1.0 \times 10^{-4}$ day$^{-1}$</td>
</tr>
<tr>
<td>Upper Floridan Aquifer</td>
<td>3</td>
<td>$Q = -353,000$ ft$^3$/day; $T_2 = 60,000$ ft$^2$/day</td>
</tr>
<tr>
<td>Middle Semi-confining Unit</td>
<td>2</td>
<td>$(K_b/b) = 5.0 \times 10^{-5}$ day$^{-1}$</td>
</tr>
<tr>
<td>Lower Floridan Aquifer</td>
<td>1</td>
<td>$T_3 = 60,000$ ft$^2$/day</td>
</tr>
<tr>
<td>Impervious Layer</td>
<td>-</td>
<td>No-flux Boundary</td>
</tr>
</tbody>
</table>

Good agreements between the simulated and analytical drawdowns of the GW head can be found in all three aquifers (Figure 4-12), revealing that CCHE3D-GW is able to simulate the pump-induced GW flows under this three-layer aquifer.

Figure 4-11. The configuration of the mesh in $x$ - $y$ plane for the simulations of the pump in the multiple-layer aquifer.
Figure 4-12. Comparisons of the drawdown computed from 3LAYSS analytical solution (Motz and Acar 2007) and simulated by CCHE3D-GW in each aquifer layer.

4.3.2 Case II: Steady State in Four-layer Aquifer

The four-layer aquifer for this verification is located in Lexmond, the Netherlands (Hemker 1985). The whole system is composed of four aquifers (Figure 4-13). For this steady state, the storativity of the aquifer ($S_i$) was zero while the transmissivity of each aquifer ($T_i$) was listed in table 4-3. The pumping well was located in Aquifer 2 and the pumping rate $Q$ was 10,000 m$^3$/day. These four aquifers are separated by confining units. For each confining unit, the ratio of the hydraulic conductivity ($K_v$) and the thickness ($b$) can be found in table 4-3. No evapotranspiration layer was set in this simulation. In the vertical direction ($z$), nine layers were set in the simulation with CCHE3D-GW where each layer was 1.0 m thick.

In the lateral plane ($x$ - $y$) the simulation domain was 290,549 m $\times$ 290,549 m which was sufficiently large to eliminate the effects from lateral boundaries. The origin of the $x$ -
The \( y \) coordinate was set at the pumping well, which was the center of the domain. The simulation domain was discretized by 293 \( \times \) 293 mesh grids in the \( x - y \) plane in which a uniform mesh \( (\Delta x = \Delta y = 30 \text{ m}) \) was used from \( x = -3000 \text{ m} \) to \( 3000 \text{ m} \) and \( y = -3000 \text{ m} \) to \( 3000 \text{ m} \), and a non-uniform mesh with the amplification factor of 1.15 was applied to the remaining domain. The lateral boundary conditions were all set to a constant head (15.0 m). The initial GW head for the simulation was set to 15.0 m.

Good agreements between the simulated and analytical drawdowns of the GW head can be found in all four aquifers (Figure 4-14), revealing that CCHE3D-GW is able to simulate the pump-induced GW flows under this four-layer aquifer.

\[
Q = -10,000 \text{m}^3/\text{day}
\]

Figure 4-13. Conceptual model of the pump in the four-layer aquifer.
Table 4-3. Hydraulic Properties of Each Layer for the Four-layer Aquifer Simulation

<table>
<thead>
<tr>
<th>Hydrogeological Units</th>
<th>Layer Number</th>
<th>Hydraulic Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top Boundary Unit</td>
<td>9</td>
<td>Constant head $H = 15.0$ m</td>
</tr>
<tr>
<td>Top Confining Unit</td>
<td>8</td>
<td>$(K_v/b) = 1.0 \times 10^{-3}$ day$^{-1}$</td>
</tr>
<tr>
<td>Aquifer 1</td>
<td>7</td>
<td>$T_1 = 2,000$ m$^2$/day</td>
</tr>
<tr>
<td>Confining Unit 1</td>
<td>6</td>
<td>$(K_v/b) = 6.67 \times 10^{-4}$ day$^{-1}$</td>
</tr>
<tr>
<td>Aquifer 2</td>
<td>5</td>
<td>$Q = -10,000$ m$^3$/day;</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$T_2 = 1,500$ m$^2$/day</td>
</tr>
<tr>
<td>Confining Unit 2</td>
<td>4</td>
<td>$(K_v/b) = 1.0 \times 10^{-3}$ day$^{-1}$</td>
</tr>
<tr>
<td>Aquifer 3</td>
<td>3</td>
<td>$T_3 = 500$ m$^2$/day</td>
</tr>
<tr>
<td>Confining Unit 3</td>
<td>2</td>
<td>$(K_v/b) = 2.5 \times 10^{-5}$ day$^{-1}$</td>
</tr>
<tr>
<td>Aquifer 4</td>
<td>1</td>
<td>$T_4 = 2,000$ m$^2$/day</td>
</tr>
<tr>
<td>Impervious Layer</td>
<td>-</td>
<td>No-flux Boundary</td>
</tr>
</tbody>
</table>

Figure 4-14. Comparisons of the drawdown computed from the analytical solution (Hemker 1985) and simulated by CCHE3D-GW in each aquifer layer.

4.3.3 Case III: Transient State in Three-layer Aquifer

The aforementioned two cases are both steady state in which the storativity is not considered. However, the temporal variation of the GW head is an important factor for designing and operating extraction and injection wells. Therefore, CCHE3D-GW is verified with a transient simulation of the pump in the three-layer aquifer described in 4.3.1.
The storativity of both aquifers and confining units shown in Figure 4-10 was considered in this simulation. The storativity values of the surficial aquifer \((S_1)\), Upper Floridan aquifer \((S_2)\) and Lower Floridan aquifer \((S_3)\) were 0.2, 0.001 and 0.001, respectively. For the confining units, the storativity was 0.01. The simulation period was around \(10^4\) days in which the first time step was \(1.0 \times 10^{-5}\) day, and the time step was multiplied by 1.2 for each of the following steps. It was found that the vertical discretization of the confining units affected the propagations of the pump-induced drawdown of the GW head (Motz and Acar 2007). As a result, three sets of mesh were tested in this verification. The first set used one layer to represent the confining units, resulting in seven vertical layers; the second set discretized the confining units by two layers, making the total number of the vertical layers nine; the third set applied four layers to representing the confining units, which in turn demanded 13 vertical layers in total.

The drawdowns of the GW head simulated by CCHE3D-GW and computed from the analytical solution (Motz and Acar 2007) were compared at the point that was 800.0 m away from the pumping well (Figure 4-15). It can be found that the agreement between the analytical and the simulated results improves when more layers are used to represent the confining unit. In addition, the agreement between the results from Motz and Acar (2007) and those from CCHE3D-GW is good, demonstrating that CCHE3D-GW can work for the transient pump in the multiple-layer aquifer.
Figure 4-15. Comparisons of the drawdown (at 800.0 m away from the pumping well) computed from 3LAYT analytical solution (Motz and Acar 2007) and simulated by CCHE3D-GW in each aquifer layer.

4.4 Verification of Variably Saturated GW Flow

The previous verification cases are all dealing with fully saturated GW flow. On the other hand, CCHE3D-GW was aimed at addressing both the deep GW and the vadose zone. Therefore, in the following subsections, the newly developed model will be verified under two variably saturated GW flow conditions. Given the complexity of unsaturated GW flows, analytical solutions are hard to find. As a result, well-accepted numerical solutions are selected for the verification.
4.4.1 One-Dimensional Infiltration

Infiltration is a prevailing phenomenon and commonly encountered for the unsaturated soil. A simple 1-D conceptualization of infiltration was chosen for verification. The scheme of the case is shown in Figure 4-16, where the domain was a 1-D soil column of 4.0 m thickness and discretized by 200 uniform mesh grid cells (Δz = 0.02 m). The initial pressure head for the whole soil was -100 m, and the z coordinate was setup downward with the origin at the land surface. The van Genuchten model was applied to describe the soil characteristic curve in which \( n = 3.45, \alpha = 1.5, \theta_s = 0.45, \theta_r = 0.05 \) and \( K_s = 0.8 \) m/day. Two time steps, \( \Delta t = 0.005 \) and 0.01 days, were tested. The total infiltration period was 1.2 days.

![Figure 4-16. Conceptual model of the 1-D infiltration case.](image)

The comparisons with the simulations of Zhang and Ewen (2000) for pressure head and moisture content distribution after 1-day infiltration were shown in Figure 4-17 (a) & (b), respectively. Good agreement can be found for these two simulation results, which indicates that the newly developed model is capable of simulating the 1-D infiltration process, particularly in capturing the infiltration front. Additionally, the fine agreement of
the results with $\Delta t = 0.005$ and 0.01 days reveals the insensitivity of the simulation to the time step under this setup.

![Figure 4-17. Comparisons between the simulation results of Zhang and Ewen (2000) and CCHE3D-GW for (a) pressure head distribution and (b) moisture content profile after 1-day infiltration.](image)

4.4.2 Single-Well Pump in an Unconfined Aquifer

Many studies have revealed that the soil properties in the unsaturated zone can affect conditions in the shallow saturated zone as well as deep GW, such as pump/injection-induced GW flow (Lin et al., 2019). However, many commonly used GW models, such as MODFLOW, ignore this component. This gap has been filled by the development of CCHE3D-GW. To verify the capacity of this newly developed model in simulating pumping with the consideration of the vadose zone, a hypothetical single-well pump numerically studied by VSAFT3 (Mao et al., 2011) is chosen.

The simulation domain was a rectangular homogeneous aquifer with the length of 200.0 m and thickness of 9.0 m (Figure 4-18). The pumping well was located at the center of the domain, and the origin was set at this point. The screen interval of the pump was
from \( z = 0.0 \) m to 4.0 m. The pumping rate was set to 0.06 m\(^3\)/min. The soil characteristic curves were represented by the model from Gardner (1958), which is written as:

\[
K(\psi) = K_s \exp(\alpha\psi) \tag{4.9a}
\]

\[
\theta(\psi) = \theta_r + (\theta_s - \theta_r) \exp(\beta\psi) \tag{4.9b}
\]

where \( \alpha \) and \( \beta \) are pore size distribution parameters, and were both set as 4.0 m\(^{-1}\) in this study. \( K_s \) is the saturated hydraulic conductivity, which is set as 0.00396 m/min. The saturated and residual moisture content, \( \theta_s \) and \( \theta_r \), was 0.37 and 0.07, respectively here.

In the \( x-y \) plane, the simulation domain was discretized by 136 \times 136 mesh grids in which a uniform mesh with \( \Delta x = \Delta y = 0.5 \) m was applied from \( x \) (or \( y \)) = -24.0 m to 24.0 m, and \( \Delta x = \Delta y = 4.0 \) m was used for the remaining domain (Figure 4-18a). In the vertical direction (\( z \)), a fine uniform mesh with \( \Delta z = 0.2 \) m was implemented for the vadose zone (from \( z = 6.1 \) m to 7.5 m), while the remaining domain was discretized with \( \Delta z = 0.5 \) m (Figure 4-18b). The lateral boundary conditions were all set to be no-flux. In the beginning, the GW table was at \( z = 6.7 \) m. The initial time step was 0.001 min, and it was amplified by a factor of 1.1 if the Modified Picard iteration could converge within five steps in the following calculation. The total simulation period was 2000 min.
The drawdowns of GW head simulated by CCHE3D-GW and VSAFT3 (Mao et al., 2011) were compared at two monitoring wells, which was 5.0 m and 30.0 m away from the pumping well in radial direction (Figure 4-19). For each monitoring well, three elevations, $z = 1.5$ m, 3.0 m and 6.0 m, were chosen for analysis. It can be found that the simulation results from CCHE3D-GW agree very well with the ones from VSAFT3, demonstrating the capability of CCHE3D-GW in accurately simulating the pump-induced variably saturated GW flows. The drawdown curves of both the saturated ($z = 1.5$ m and 3.0 m) and vadose zones ($z = 6.0$ m) follow a three-phase shape indicitative of differing water release mechanisms of compressibility and drainage. The drawdown of the saturated zone is larger than the unsaturated zone, while within the saturated zone the drawdowns are generally the same when comparing $z = 1.5$ m and 3.0 m.
Figure 4.19. Comparisons between the simulation results of VSAFT3 (Mao et al., 2011) and CCHE3D-GW for drawdowns at different elevations where the monitoring well is (a) 5.0 m and (b) 30.0 m away from the pumping well in radial direction.
CHAPTER 5 Conclusions

The CCHE3D-GW model has been developed for simulating variably saturated GW flows, making it capable of handling flows in both fully saturated soil and the vadose zone. Various boundary conditions for GW flows, such as active wells (pumping or injection), general-head condition and flux boundary condition, have been developed as modules in CCHE3D-GW. In the present version of CCHE3D-GW, the SW dynamics, such as stream flow, are considered as boundary conditions. As a result, the GW-SW interactions are simulated by simplifying SW flows to be head or flux boundaries. Although CCHE3D-GW has not been integrated with the NCCHE SW models (CCHE2D/3D), the framework of this model is the same as that adopted in CCHE2D/3D, making it easier to develop an integrated GW-SW model in the future. Some new functions, such as considering time-varying streambed conductivity and aquifer hydraulic conductivity, have also been incorporated into CCHE3D-GW.

In the development processes, CCHE3D-GW has been verified with analytical solutions and many sets of published numerical solutions. Good agreement between the results computed by analytical/numerical solutions and the ones simulated by CCHE3D-GW demonstrate the correctness, robustness and applicability of this newly developed model.

In summary, CCHE3D-GW has been proven accurate and efficient in simulating variably saturated GW flows. It can serve as a useful tool to help the decision-making for the GW resources management.
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